ADVANCED COMPUTATIONS & MODELING FOR NONLINEAR & STOCHASTIC WAVES

FINAL REPORT

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August 9, 1995

U. S. ARMY RESEARCH OFFICE

DAAL03-92-G-0185

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Foreword

The goal of this project was to address basic nonlinear problems in the modeling of physical systems with engineering relevance. Nonlinear conservation laws were chosen for study because these differential equations are basic to many applications. We also studied stochastic issues, as they are often of great importance in nonlinear modeling of physical phenomena. In these studies, we used mathematical theory, first principle computations and analysis of experimental and field data.

Motivating applications of our work included, inertial confinement fusion, shock and gravity induced fluid mixing, fluid jet breakup. ground water flows, petroleum reservoir modeling, and high velocity impacts. Additional applications included vehicle signature identification (radar cross sections), advanced manufacturing technology, pharmacology and drug activity through protein-DNA binding studies, and remediation of environmentally polluted facilities.

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1. RESEARCH SUMMARY

1.1. Global Solutions to the Compressible Euler Equations with Geometrical Structure. Joint work with G.-Q. Chen [Chen and Glimm, 1994a, Chen and Glimm, 1994b] settled a theoretical question that has been outstanding for several decades, namely how to control the influence of reflected waves from infinity, to prove existence theorems for the Euler equations of isentropic gas dynamics for radially symmetric flow in two and three dimensions. The domain considered, $r \geq 1$, includes the singularities associated with infinity, but excludes the singularity of focusing at the origin. The main idea in the proof, which uses the compensated compactness framework, is to construct approximate solution operators and approximate Riemann solutions that incorporate leading order radial corrections. These are based on exact solutions of the radial equations which are steady, i.e. no with no time dependence.

1.2. Stochastic Analysis of Fluid Waves. Macroscopic behavior is the result of averages over small scale fluctuations. Ensemble averages are a convenient formalism to express this principle. Ensemble averages introduce the severe complication of function space integrals, or of analysis in infinite dimensional function spaces. Such difficulties are also encountered in statistical physics and quantum field theory [Glimm and Jaffe, 1981]. We used four methods to study ensemble averages: renormalization group methods, moment expansions, perturbation theory (ordinary and renormalized), and direct numerical simulation.

1.2.1. Renormalization Group Analysis. In the renormalization group (RNG) approach, there is a continuum of length scales, with integration over all small scales used to define the effective equations on some intermediate length scale. The introduction of new (small) length scales and the change in location of the intermediate length scale is treated differentially, to give the renormalization group equation. The case of a fixed point for this equation is of special interest. In this case, the problem formulation and equations do not change as the intermediate length scale is varied. The equations and solutions are self similar. Power law exponents and premultiplying coefficients then determine the solution. Usually the exact integration of the small length scales gives rise to extremely complicated effective equations, which are difficult to work with. Fortunately, in the case of a fixed point, approximations will not change the exact answer. The fixed point will normally be stable to perturbations, or at least to many of them. Let us call the stable perturbing directions for the equations of motion irrelevant, and the unstable directions, relevant. Then any irrelevant terms in the exactly integrated effective equations can be discarded. The effective equations at the intermediate length scale will contain only relevant terms. The three step renormalization group process is as follows: integrate a (differential) unit of length scale dk, rescale, so that the equations are formulated at a constant length scale, and finally truncate, so that irrelevant terms are dropped. If this process yields the identity, so that the equations do not change under integration of length scales, then a fixed point has been found.

We have use a variant of this method to study the Rayleigh-Taylor fluid mixing process. This mixing process is an acceleration driven instability of an interface separating fluids of different densities. We wish to characterize the height

$$h = \alpha A g t^2$$

of the mixing zone as a function of time. t, where g is the (gravitational) acceleration, $A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$ is the Atwood number, a buoyancy renormalization of g, the ρ_i are densities on the two sides of the interface, and α is a dimensionless constant that characterizes the mixing rate. For incompressible flows, $\alpha = .06$ is a universal constant. An unusual feature of this problem is that the time evolution enforces dynamically a change (increase) of the effective length scale. Thus time can be taken as the otherwise artificial parameter in the renormalization group equation dynamics.

The temporal dynamics coincides with the renormalization group dynamics and the renormalization group describes the transients, *i.e.* the dynamical approach to steady state self similarity. We feel that this is an important observation, that may find validity in many related "totally unstable, unstable on all length scales" instabilities, such as the Taylor-Saffman, Kelvin-Helmholtz, and metastable phase transition instabilities.

Our RNG study of the Rayleigh-Taylor instability starts with a modification of the Sharp-Wheeler model, and defines a statistical model for the dynamic evolution of an ensemble of bubbles. This model is regarded as an approximation to the two fluid Euler equations, describing the fluid evolution directly. The bubble model has its own laws of dynamical evolution. Each bubble moves as the sum of two velocities. The first is due to the bubble itself, and is the terminal velocity taken from single bubble studies of the Rayleigh-Taylor problem. It is a function of the bubble width. The second contribution is a velocity associated with the bubble interactions, and is defined in terms of the relative position of the bubble and its neighbor. It is also derived from single bubble studies of the Rayleigh-Taylor problem. At sufficiently large relative heights, a merger process will occur between adjacent bubbles, leading to a new bubble, of width equal to the combined widths of the two that are merging. The parameter in the model that controls merger is set from numerical Rayleigh-Taylor studies of two adjacent bubbles, and checked by analysis of experimental data. This model [Glimm and Sharp, 1990, Glimm et al., 1991], is then approximated. First, the adjacent bubble interactions are approximated by random pairs selected from the ensemble, and then the probability distributions for the bubbles are approximated by a specific parametric form. The dynamics is then projected into a dynamics for the parameters of the bubble probabilities. This dynamics is the renormalization group equation, and a fixed point is found. Further analysis showed that this fixed point is in quantitative agreement with the growth rate of the mixing zone, as determined experimentally [Read, 1984, Youngs, 1984a], and computationally, by the front tracking method [Zhang, 1990].

In this application of the renormalization group method to the Rayleigh-Taylor problem, we did not analyze relevant and irrelevant terms. Rather we followed the methods of intuitive physics to justify the approximations. Our approach has the benefit that each intermediate step has a physical interpretation. To compensate for the omission, an independent check on the conclusions was required, which we supplied in the form of agreement of the RNG fixed point behavior with experimental and numerical simulation data.

1.2.2. *Moment Expansions.* In moment expansion methods, dynamical equations are derived for low order moments of the ensemble average [Drew, 1983, McComb, 1990]. Equation nonlinearities couple low order moments to higher ones, and a closure hypothesis is needed to complete the dynamical equations. This hypothesis is not to be "derived" in a mathematical manner from existing laws of physics, but is to be "introduced" as a physical principle on its own merit. Thus it must be justified by appeal to measured or simulated data, and its use must be restricted to regimes for which it is valid. Usually the limitations of the moment expansion method lie in this step of validation and restriction.

We have applied the moment expansion method to the study of the Rayleigh-Taylor mixing layer. Our preliminary results are:

(a) A two phase description fits the data better than a turbulence description.
(b) A new first moment two phase closure is proposed.
(c) A one parameter family of solutions is obtained to the ensemble averaged equations.
(d) A better understanding of the loss of universality for the compressible Rayleigh-Taylor mixing phenomena is achieved.
(e) The new equations are hyperbolic. *i.e.*, they have purely real characteristics.

We also note earlier work [Stewart and Wendroff, 1984] in which purely hyperbolic multiphase equations are proposed.

The new two phase ensemble averaged equations have the form:

$$\frac{\partial \alpha_k}{\partial t} + (\alpha_1 \bar{v}_2 + \alpha_2 \bar{v}_1) \frac{\partial \alpha_k}{\partial z} = 0 \ ,$$

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \frac{\partial \alpha_k \bar{\rho}_k \bar{v}_k}{\partial z} = 0 \ ,$$

$$\frac{\partial \alpha_k \bar{\rho}_k \bar{v}_k}{\partial t} + \frac{\partial (\alpha_k \bar{\rho}_k \bar{v}_k \bar{v}_k)}{\partial z} = -\frac{\partial (\alpha_k \bar{p}_k)}{\partial z} + \alpha_k \bar{\rho}_k g$$

$$+ (\alpha_1 \bar{p}_2 + \alpha_2 \bar{p}_1) \frac{\partial \alpha_k}{\partial z} \ ,$$

$$\frac{\partial (\alpha_k \bar{\rho}_k \tilde{\epsilon}_k)}{\partial t} + \frac{\partial (\alpha_k \bar{\rho}_k \tilde{\epsilon}_k \bar{v}_k)}{\partial z} = -\bar{p}_k \frac{\partial (\alpha_k \bar{v}_k)}{\partial z} + (\alpha_1 \bar{p}_2 \bar{v}_2 + \alpha_2 \bar{p}_1 \bar{v}_1) \frac{\partial \alpha_k}{\partial z} \ ,$$

for $k = 1, 2$ and

$$\alpha_1 + \alpha_2 = 1 \ ,$$

where α_k is the volume fraction, bars denote volume weighted averages, and tildes denote density weighted averages, ρ is density, v is velocity, p is pressure, g gravity and ϵ is the internal energy. See [Harlow and Amsden, 1975, Youngs, 1984b, Freed et al., 1991] for a discussion of equations (derivable from the above) in which there is a single equilibrated pressure, and the flow is incompressible.

We studied both turbulence and two phase descriptions of this mixing data, as both have been proposed for this problem. We derived an identity to write the second order turbulence moments such as the Reynolds stress as products of the first order two phase moments, plus an intrinsic two phase second order turbulence contribution. The latter was seen to be negligible in the Rayleigh-Taylor data we analyzed. This fact supports our conclusion that the two phase description is more appropriate for this data [Chen et al., 1995].

1.2.3. *Perturbation Theory.* The method of perturbation theory is useful for small random fluctuations. Together with coworkers, we applied both ordinary and renormalized perturbation theory to the problem of transport by a random velocity field.

The transport of a passive (noninteracting) scalar contaminant u by a random velocity field $\vec{v}$ arises in environmental studies of ground water. The equation governing this flow [Dagan, 1989] is

$$u_t + \vec{\nabla} \cdot \vec{v} u = 0 \ .$$

Here $\vec{v}$ is a Gaussian random field, defined in terms of its covariance, $\langle \vec{v}(x), \vec{v}(y) \rangle$. We assume that the statistics are stationary, self similar (fractal), isotropic and incompressible. More generally, random fields with stationary increments [Gelfand and Vilenkin, 1964, Yaglom, 1986] have been used to model geostatistics; in some approximation, these random fields describe the velocities as well. It follows that the covariance has a power law form, as a function of $r = |x - y|$, namely $br^{-\beta}$. Since $\vec{v}$ is a random field, so is $u = u(x, t)$, and the problem is to relate the statistics of $\vec{v}$ to that of u. The stochastic property of $\vec{v}$ reflects the lack of knowledge of details of small scale variations in the geology, and hence in the ground water flow velocity, $\vec{v}$. We write $v = \bar{v} + \delta \vec{v}$, where $\bar{v} = \langle \vec{v} \rangle$ is the ensemble average, or mean flow. Perturbation theory expresses u as a series in powers of $\delta \vec{v}$. The leading order contribution to u resulting from statistical fluctuations $\delta \vec{v}$ in $\vec{v}$ is a diffusion term, added to the transport of $\bar{u}$,

$$\bar{u}_t + \nabla \cdot \bar{v} \bar{u} = \nu \Delta \bar{u} \ ,$$

where

$$\nu = \int \langle \delta \vec{v}(x + \bar{v}t) \delta v(x) \rangle dt \ .$$

In the case of slowly decaying velocity correlations the dispersion is anomalous, *i.e.* not Fickean, and $\bar{u}$ is a solution of the diffusion equation with a time dependent diffusion constant. Anomalous diffusion is consistent with field data, for ground water flow, for which it is known that the dispersion coefficients increase with time or travel distance [Gelhar et al., 1985], by up to six orders of

magnitude. Our analysis traced this anomalous aspect of the dispersion in ground water flows to slowly decaying correlations in the geological data, specifically to the correlations of permeability, and hence to the velocity field, in our models. Our main conclusion is that a self similar, or fractal description of the velocity field leads to mixing behavior that is not self similar, but whose short and long distance limits have (different, but explicitly determined) scaling laws. Let the mixing length l be a function of the travel distance L. An asymptotic scaling law states that $l \sim L^{\alpha}$. The scaling law $\alpha = 1/2$ is Fickean, and is valid for large L if $\beta > 1$, *i.e.* if the integral defining ν above is convergent. Otherwise, the diffusion is not Fickean, and, in general,

$$\alpha = \max\left\{\frac{1}{2}, 1 - \frac{\beta}{2}\right\}.$$

For ground water problems, the transient *i.e.* preasymptotic dispersion is more important than the asymptotic dispersion. See [Furtado et al., 1992, Glimm et al., 1992, Glimm et al., 1993a].

1.3. Computation. Recent developments have enabled our front tracking code to compute successfully several problems of long standing, leading to greatly improved computations and, for some cases, a first correct computation. These new capabilities are also laying the groundwork for new fundamental studies in the future.

1.3.1. *Stochastic Flows.* The method of direct numerical simulation is a powerful tool for the analysis of stochastic theories. It provides data for assessing the validity of approximate theoretical models and it provides solutions for which there is no applicable theory. We have studied the two problems introduced above by this method: the Rayleigh-Taylor problem and the anomalous diffusion due to transport by a random velocity field. Both studies focused on the growth rate of the mixing zone. For the Rayleigh-Taylor problem, we have the only compressible computation which shows agreement with incompressible experiments in the incompressible limit. (There is no compressible experimental data available.) We discovered, on the basis of computational experiments, a loss of universality for the growth rate in the compressible case, and a possible doubling of the growth rate [Chen et al., 1993, Deng et al., 1993]. In more recent work, we obtained an understanding of the loss of universality, or ensemble dependence of the growth rate. It appears that the initial instability amplitude, or the relative amplitudes of the long and short wave lengths in the initial data are significant variables for the growth rate determination [Chen et al., 1995].

Our simulations displayed anomalous dispersion in agreement with both ordinary and renormalized perturbation theory solutions, for transport by a random velocity field [Furtado et al., 1992, Glimm et al., 1993a].

In [Li et al., 1995] we compared front tracking to TVD schemes, with and without artificial compression. The latter was also discussed in three dimensions. It was found that TVD is diffusive for the Rayleigh-Taylor problems, and that this problem was to a large extent overcome by the use of artificial compression. The level set method, also used in this study, is a post processing step, and affects the graphical output, but not the computation.

1.3.2. *Shock Diffraction.* The first of these new developments is the use of front tracking for shock wave diffraction by a fluid interface or by an obstacle. The novelty is not the principle of such a front tracking computation, which was first achieved by the proposers and coworkers some years ago, but its robustness. Robustness is measured by the number of cases handled automatically, or by the complexity of the problems thus solved automatically. The computations are based on shock polars, which are equations defined by shock wave jump conditions, composed in sequence for all the waves meeting at a point. As a tool for graphical understanding, the shock polars are projected on some convenient plane (such as the pressure, turning angle plane). We use shock polar analysis as a constructive numerical step in our front tracking finite difference code. The analysis inserts analytic information into the computation where it is most needed, at the points of greatest computational difficulty. The result of this method are computations of remarkable accuracy, often

on very coarse grids. The dynamic change of the topology defined by the fronts is automated to allow the formation of new shock waves. and the elimination of others as they disappear from the computation or become less important. The hierarchy of possible shock diffraction diagrams is exceedingly complex, and not all of them are presently supported as front tracking capabilities. Rather, support for enough of them has been achieved to allow solution of various interesting problems. Validation studies for a regular Mach reflection, computed by these methods, have been reported [Boston et al., 1993b]. One interesting flow pattern studied was the height of burst problem for the interaction of an expanding spherical shock wave with a thermal boundary layer above a planar rigid surface, see Figure 1.1.
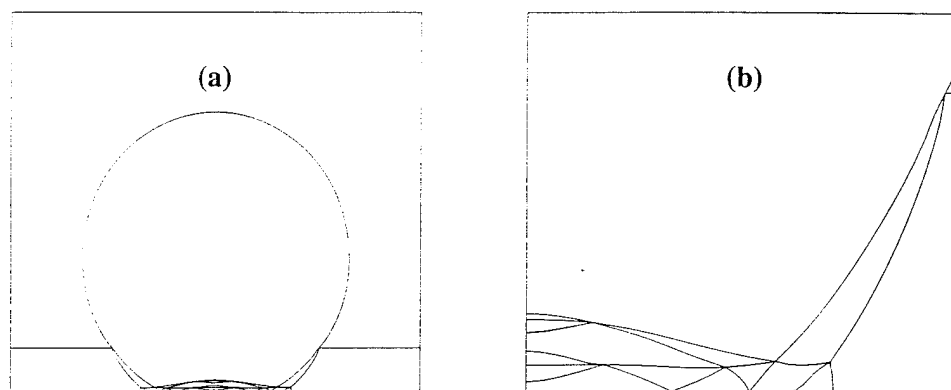

FIGURE 1.1. The tracked fronts for the height of burst problem with a thermal boundary layer. (a) shows the entire grid, and (b) a blow up of the lower right portion of the grid. The vertical coordinates have been stretched by a factor of 67% in (b). The grid is 50 × 50, so that the boundary layer is exactly five mesh zones in width. The frame (b) occupies a 6 × 6 grid subregion of the full computation.

Another interesting study concerned the regular reflection – Mach stem transition. Computations with wedge angles within a fraction of a degree of the von Neumann transition angle were obtained. The best comparison computation (based on Godunov methods, local mesh refinement and a limited version of front tracking) [Henderson et al., 1993] required considerably more resources to obtain a less precise determination of the transition point. The two computations agreed within their common domain of definition. See Figure 1.2.

The most important application of this enhanced front tracking shock wave diffraction capability is to shock induced turbulent mixing, described below.

1.3.3. *Parallelism.* The second recent development for front tracking is its extension to parallel MIMD hardware. This extension has enabled most of the other computations reported here. For hyperbolic conservation laws, with explicit time step integration, domain decomposition is implemented with use of "ghost cells" to extend the size of each domain by approximately one-half of the stencil width. The data from the ghost cells allow the ordinary serial code to compute for a time step on each domain. At the end of the time step, communication is used to update the ghost cells, as a block. In this method, communication is restricted to data proportional to the boundary of the domains, and the number of communication packets is $O(1)$. A complication of front tracking, for this algorithm. is its extensive use of the C language data structures, including function and data pointers. After communication, the data pointers are incorrectly set, and must be reset through controlled storage allocation within designated storage blocks and through pointer arithmetic, to generate the offset in relative addresses between distinct blocks. In addition, a number of previously solved problems. such as the remeshing of points on the front, had to be reexamined, since the previously used global algorithm of uniform spacing by arclength is not convenient relative
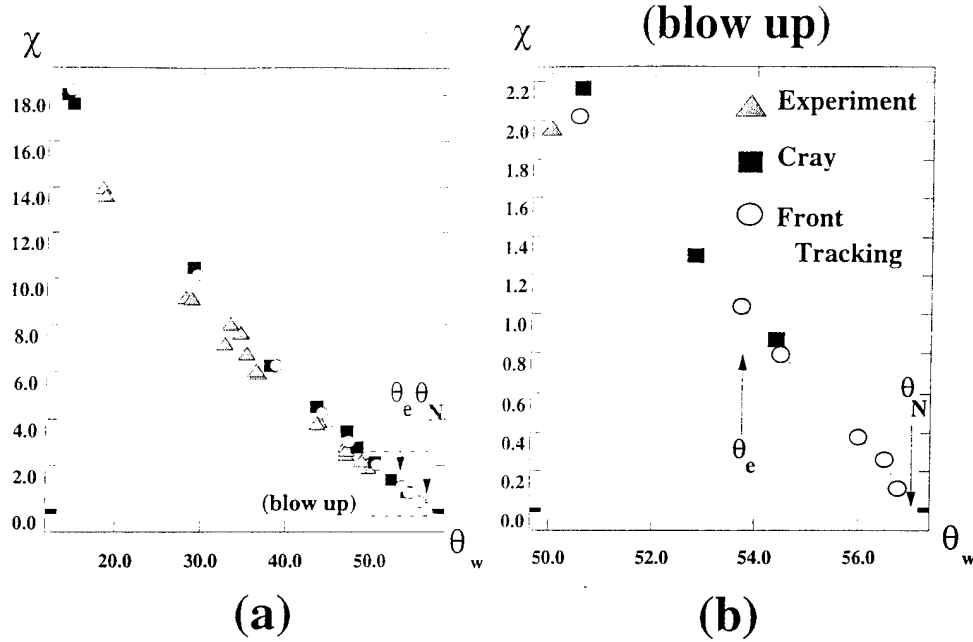
FIGURE 1.2. Graphs of the ramp angle θ_w vs. the trajectory angle of the Mach node, χ. θ_e is the detachment angle, beyond which regular reflection is theoretically impossible, and θ_N the mechanical equilibrium or von Neumann point. The experimental results can get no closer to transition than seven degrees, and the CRAY results no closer than three degrees. both due to a lack of resolution near the wall. The front tracking results represent resolution to within one half degree of transition.

to one which is local to each processor. The parallelization has been a success by all measures: The parallel speed up is above 90%. The time spent in communications is small relative to the time spent in computations. The results produced are of considerable scientific interest, and could not have been obtained without the parallelization. The level of utilization of our local parallel hardware approaches 100%.

1.3.4. *Three Dimensional Front Tracking.* The third recent development is the extension of front tracking to three dimensions. This extension is still undergoing validation studies, and a paper describing its capabilities is being prepared. See also [Li et al., 1993, Glimm et al., 1995a]. We discuss in detail here one subroutine of this program, namely the efficient interpolation of piecewise smooth data in three dimensions. The front tracking interface structure will support the description of an arbitrary set of discontinuity surfaces. intersecting along curves, which themselves intersect on codimension three objects, *i.e.* points. and referred to here as nodes. The interface structure is represented discretely as piecewise linear objects. Thus the discretized surface is composed of triangles, and the curves are composed of line segments, called bonds. The two ends of the line segments (bonds) are called points. The vertices of the surface triangles are also called points, and for surfaces meeting in a common curve. there will also be triangles meeting at a common bond. Geometrically identical points are shared as a common object. The surface is oriented, so that a distinguished normal direction (positive) is introduced. At each point there is a positive and a negative storage location for discontinuous solution state variables. Along curves, where multiple surfaces meet, states are stored for positive and negative sides of each surface bounded by the curve, at each point (bond start or endpoint) of the curve. In addition, state variable storage is provided at all regular grid locations, at grid cell centers. The interpolation problem is to construct an

efficient solution function that will return an interpolated solution at an arbitrary location in three dimensional space, and that is guaranteed robust, in the following two senses: The discontinuity interface will divide space into connected components. If the connected component is specified, then the interpolation is guaranteed to be among grid cell values associated with this component only. If no component is given, then the component associated with this location will be computed efficiently, and the previous method used.

Efficient precomputation of components and their storage on those grid cells not meeting the interface (so that they are uniquely defined) is accomplished by a hashing method, which lists all triangles meeting a given mesh cell. From this list, an $O(1)$ computation will give local component information. This local information can be propagated to nearest neighbors, if there is no intervening interface, and thus extended to all of the computational domain. The evaluation of the robust solution function uses the dual grid, with data located at grid corners, not at grid cell centers. Evaluation is by bilinear interpolation for points lying in regular dual grid cells. For grid cells meeting the interface, a further tetrahedralization is needed. Because the tetrahedra will be used for linear interpolation, no new interior vertices (at which there would be missing data) can be introduced. It is known that the above problem is in general insoluble, unless new points are introduced. In fact, it would be possible to introduce new points on the interface, giving it very small triangles. Data at the new triangular points would be obtained by linear interpolation on the original triangles. This solution is not very desirable, as it appears to be computationally inefficient. Instead, we use a Dulaney tetrahedralization of space. This tetrahedralization will not respect the division of space into components by the interface. In other words, an individual tetrahedron, with vertices defined by one component, may intersect another component. Thus we divide our data points into the components they represent, and construct an independent tetrahedralization for each component. For efficiency reasons this is done locally within each dual grid mesh block. Since the interpolating function is to be supplied with a component as an argument, or by a side computation, it will call up the interpolation based on the Dulaney tetrahedralization of that component.

1.3.5. *E&M Scattering Cross Sections.* We also developed a two step multigrid algorithm for the solution of electro-magnetic scattering problems by boundary integral methods. These problems are memory limited, and since only the coarse grid inverse matrix is stored (the fine grid direct matrix is computed on the fly, using tabulated, efficient special functions), problems up to 25 times larger than normal (single step) methods can be solved by this algorithm. We also investigated limitations of this algorithm, associated with resonances. For dielectric material, and also for indentations in a perfectly conducting plane surface, the problem of resonances was overcome. The algorithm was implemented as MIMD parallelized code. On a small parallel computer, we are able to solve 30.000 equations using a two level iterative approach, for dielectric materials and for indentations in a plane surface [Asvestas et al., 1993, Asvestas et al., 1994]. This same code has been adapted to solve radiative heat transport problems, for application to crystal growth modeling. Heat transport is of interest to us as a detail in a planned integrated approach to the modeling, design, and manufacturing control of the crystal pulling process.

1.4. Applications.

1.4.1. *Shock Induced Mixing.* The proposers and coworkers have recently obtained significant progress in understanding turbulent mixing and multiphase flow. Our efforts have been concentrated on acceleration induced instabilities of an interface between fluids of differing densities. The case of impulsive acceleration, as due to a shock wave, is known as the Richtmyer-Meshkov instability; the case of steady acceleration, as due to a gravitational force, is known as the Rayleigh-Taylor instability.

The agreement obtained (for the first time) between computation and experiment in the growth rate of the Richtmyer-Meshkov instability [Grove et al., 1993a, Grove et al., 1993c, Grove, 1994,

Grove et al., 1993c, Boston et al., 1993c, Boston et al., 1993a] is the most important aspect of the progress reported here. In Figure 1.3a we show the growth rates for a Richtmyer-Meshkov instability, determined by a front tracking simulation. Superimposed on this plot is the growth rate reported from experiment [Benjamin et al., 1993], that obtained by linear perturbation theory, and the growth rate of the Richtmyer impulsive model.

These computations have produced a far deeper understanding of the theory of this instability than has been previously available [Boston et al., 1995a, Grove et al., 1995, Holmes et al., 1995, Boston et al.. 1995b]. We understand the shock diffraction mechanisms that yield the decay in the mixing growth rates. In Figure 1.3b-e, we show plots of pressure at the times corresponding to the down turns in the growth rate, as shown in Figure 1.3a. Note the appearance of a pressure pulse at either the peak or the trough of the mixing interface in these figures, to cause a sudden dip in the growth of the peak to trough separation. The pressure pulses originate in the intersection of curved shock waves, moving transversely to the interface and coming from the curvature of the original interface.
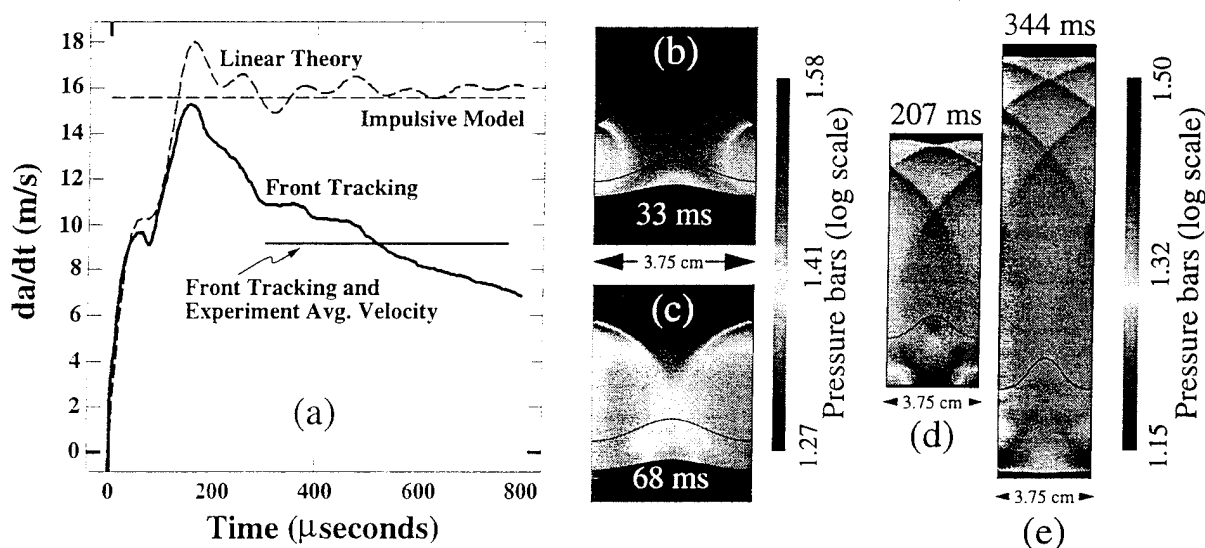
FIGURE 1.3. (a) The amplitude growth rate, $\dot{a}(t)$, of a shocked air-SF_6 interface. This graph compares the results of experimental averages, front tracking simulation, linear theory and Richtmyer's impulsive model. Also shown are results of a least squares fit to the front tracking amplitude data over the period of experimental observation. (b-e) Pressure plots at a series of times for the nonlinear air-SF_6 solution. A cascade of shock waves generated by the self-interaction of the transmitted and reflected waves propagate back toward the interface and affect the perturbation growth rate at early and intermediate times.

We also understand the failure of other computations to give the right answer: numerical diffusion of the interface led to a diminished shock-interface interaction. The numerical diffusion becomes more pronounced as the computation progresses, so that the effects of moderate or late time shock-interface interactions were especially diminished. However, it was these late time interactions, due to reflections from the curved contact discontinuity and the curved shock waves, that caused the decay in the growth rate of the instability. Lagrangian computations [Meyer and Blewett, 1972], with a sharp fluid interface, were not carried to late time, presumably due to mesh tangling problems. An incorrect physical picture, corrected in work of the proposers and coworkers cited above, held that the growth rate for the instability was constant in time. This picture led to inappropriate

comparisons between growth rates, for example between those observed at different time intervals, and it led to the recording of a single growth rate in experiment, rather than the recording of the growth history over the longest possible observable interval.

Other computations had reasonable performance for early time growth rates, but they developed inaccuracies before the period of experimental observations began and displayed errors in over predicting the growth rate during the experimentally observed period, typically by a factor of two. Popular theoretical models for prediction of this instability also give incorrect answers, and the basis for these discrepancies is now understood. Fundamentally, these methods are based on small amplitude assumptions and linearization of the perturbation of an idealized flat interface. This assumption is invalid for the times and instability amplitudes considered.

1.4.2. *Resin Transfer Molding.* Resin Transfer Molding (RTM) is a process to produce light weight, high strength structural components, possibly with complex geometries, for aerospace and automotive applications. In this process, a liquid plastic resin is injected under pressure into a woven mat of carbon fiber; the part is then set, or hardened, by curing, *i.e.* polymerization of the resin, by baking it in an autoclave. There are many variations on this process, for example in which the resin sets chemically during the injection process rather than during a separate thermal stage. As a new manufacturing process, there are many unresolved technical issues, a number of which are under active study. Representative issues include the strength and durability of the finished part, residual stresses and warpage resulting from thermal gradients induced during cure, and the design of the fill process itself. Within the latter, important process variables include the fill rate (*i.e.* the driving pressure gradient), the capillary number, the resin-fiber wettability, the contact angle, the fiber mat characteristics, the uniformity of the fiber fill, especially at corners and edges, and the location of the inlet/outlet ports and their driving pressure histories.

Among the important issues these variables seek to control is the possible formation of large areas not contacted by resin (dry spots). Dry spots have a catastrophic influence on strength and result in an unacceptable product. Also very significant is the control of small voids, or microbubbles, that can reduce strength by a factor of two.

The mathematical analysis of RTM is described at the continuum level by Darcy's law

$$v = -\lambda \nabla P \ , \ \nabla v = 0 \ ,$$

where v is the velocity of the resin as it is injected through the fiber mat, P is the driving pressure, and $\lambda = K/\mu$ is the transmissibility, with K permeability and μ resin viscosity. The injection is usually modeled as a free boundary problem, with the resin front moving at the above Darcy velocity.

A number of authors have studied the microflow properties of resin moving around and between fibers twisted into a string, or "tow", around the tows woven into a mat, and between the mats pressed in layers into the mold form [Aström et al., 1992, Bayramli and Powell, 1992, Chen, 1993]. In general there has been little study connecting such microflow issues to continuum level descriptions such as a Darcy's law flow description or a predictive manufacturing design capability to select or control the various process variables for optimization of manufacturing design. This is precisely the issue we have addressed.

The investigators and coworkers, in collaboration with a manufacturing research team from Northrup-Grumman, initiated such a study, with the specific goal of identifying the process variables that would allow reduction of microvoids. A preliminary study was completed [Chui et al., 1995a]. The study used a new continuum level description of the flow process. Following the ideas of porous media flow, a relative as well as an absolute permeability was introduced, to model the flow properties of the microbubbles. Thus we consider the Buckley-Leverett equation [Lake, 1989]

$$s_t + \nabla \cdot v f(s) = 0 \ .$$

Here s is the volume fraction of the void space occupied by the injected resin, v is the velocity from Darcy's law above, and f is a fractional flow function, that expresses resin flow as a fraction of total (resin and air) flow. f is expressed directly in terms of the relative permeabilities, $k_i(s)$, $i = a$ (air) or $i = r$ (resin), and

$$f = \frac{k_r/\mu_r}{k_a/\mu_a + k_r/\mu_r} \; ,$$

while λ above is replaced by

$$\lambda = \left(\frac{k_a}{\mu_a} + \frac{k_r}{\mu_r} \right) K \; .$$

We use a standard quadratic form $k_r = s^2$ for the resin relative permeability, but the air relative permeability, $k_a = (s_R - s)^2$ if $s < s_R$ and $k_a = 0$ otherwise, is a quadratic as a function of the reduced saturation defined in terms of a residual air saturation s_R. We take s_R to be pressure dependent to express a higher mobility of the microbubbles at increased pressure, to allow for reduced volume of the (compressible) bubbles in a higher pressure field.

The resulting flow simulations [Chui et al., 1995a, Chui et al., 1995b] were shown to agree quantitatively with experiments performed in Sweden [Lundstrom and Gebart, 1992], see Figure 1.4.

Void Distribution at Breakthrough

Outlet Pressure: 1 atm

Void Fraction (%)
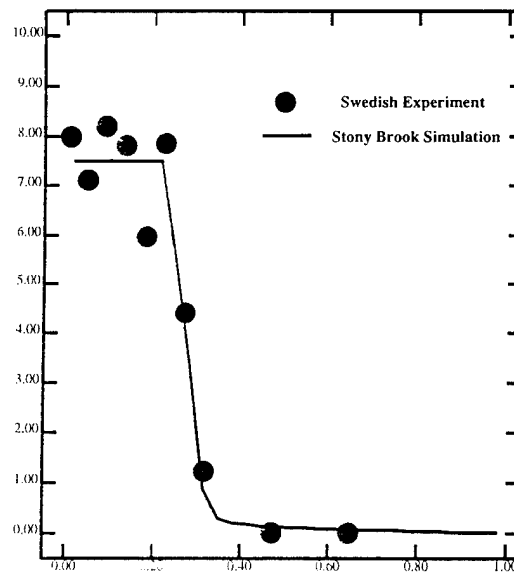
Normalized Distance to Outlet

FIGURE 1.4. In the experiments the mold was filled till "breakthrough", after which time the resin cured and the void distribution was measured along the mold. The voids concentrate on the outlet side of the mold. Our relative permeability models have a few physical parameters. The figure shows that these parameters can be adjusted to give quantitative agreement between experiment and simulation.

The most important flow variable for the control of microvoids in these experiments was the evacuation level of the mold during filling. Similar experiments were performed at Northrup-Grumman, reaching the same conclusion. It was found that components of excellent quality were produced at sufficient level of evacuation of the mold prior to the resin injection.

1.4.3. *Elastic Plastic Deformations.* The proposers and coworkers have suggested a new approach for the computational modeling of elastic plastic deformation [Glimm et al., 1993b]. This effort is intended to allow improved simulations for large deformation problems, as occur in penetration mechanics, tool cutting, punching, and other metal forming processes. The new methods proposed are useful either individually or in combination. The principle components of our approach are (a) a fully conservative, Eulerian, upwind finite difference approach with (b) material models based on a hyperelastic strain energy, (c) front tracking, (d) improved physics modeling for rate independent plasticity, and (e) special modeling to allow tracking of shear bands [Glimm et al., 1995b]. The fully conservative Eulerian formulation [Plohr and Sharp, 1989, Plohr and Sharp, 1992] has been completed, and represents the first occasion in which fully conservative equations have been written for plastic deformation (or even for the Eulerian formulation of elastic deformation). In the case of plasticity, the equations contain new physical principles, as the conservative formulation implies jump conditions not contained in nonconservative formulations. These two formulations are equivalent for smooth flows only. The conservative independent variables are strain quantities, as opposed to the nonconservative stresses usually used as primitive variables. The formulation is Eulerian, so that Lagrangian mesh tangling will not arise, even in the case of large deformations. In some Lagrangian codes, mesh tangling is avoided by use of the method of erosion. In the erosion method, mesh cells are simply removed from the computation, together with the material contained in them, when they become too tangled or too distorted to allow the computation to continue. The approach we propose will use mesh and interface constructions consistent with recognized physical principles.

The fully conservative formulation requires a hyperelastic equation of state, in which material properties such as stress are represented as partial derivatives of a thermodynamic strain energy. The hyperelastic formulation is not conventional in the materials modeling community, in contrast to incremental, or hyperelastic thermodynamics, in which thermodynamic quantities are obtained from the solution of differential equations. In contrast, the modeling of fluids has been based almost exclusively on a hyperelastic, or strain energy based equation of state for several decades. To formulate the hyperelastic strain energy, we follow conventional ideas, and use a small deviatoric shear model [Garaizar, 1989] in which the isotropic, or fluid equation of state is obtained from conventional fluid ideas, such as a stiffened gamma gas law or a tabular equation of state [ANO,] and the deviatoric shear strain energy is added perturbatively, as a quadratic correction to the isotropic energy. In this we follow conventional ideas, *cf.* Steinberg and Lund [Steinberg and Lund, 1989]. Validation is required, due to the change from a hyperelastic (nonconservative, incremental) equation of state model to a hyperelastic one [Wang et al., 1993a].

Some of the material constants for rate dependent plasticity can be obtained by direct measurement, while others are inferred only indirectly by the agreement between one dimensional plate impact computations and experiments. In the process of the validation study, we found a deficiency in the original physics model and its numerical implementation, which implicitly set the plasticity to be rate independent for strain rates exceeding the Peierls threshold. This physics modeling assumption, which is not consistent with general ideas of physics, was not stated clearly as a condition of the model, but was an incidental aspect its implementation. This model seems to be replicated in several plasticity production codes. An improved physics model was proposed, and agreement between the conservative *vs.* nonconservative, and hyperelastic *vs.* hyperelastic formulations was obtained [Grove et al., 1993b, Wang et al., 1995]. Agreement between simulation codes based on two different plasticity formulations means that the material parameters that allowed
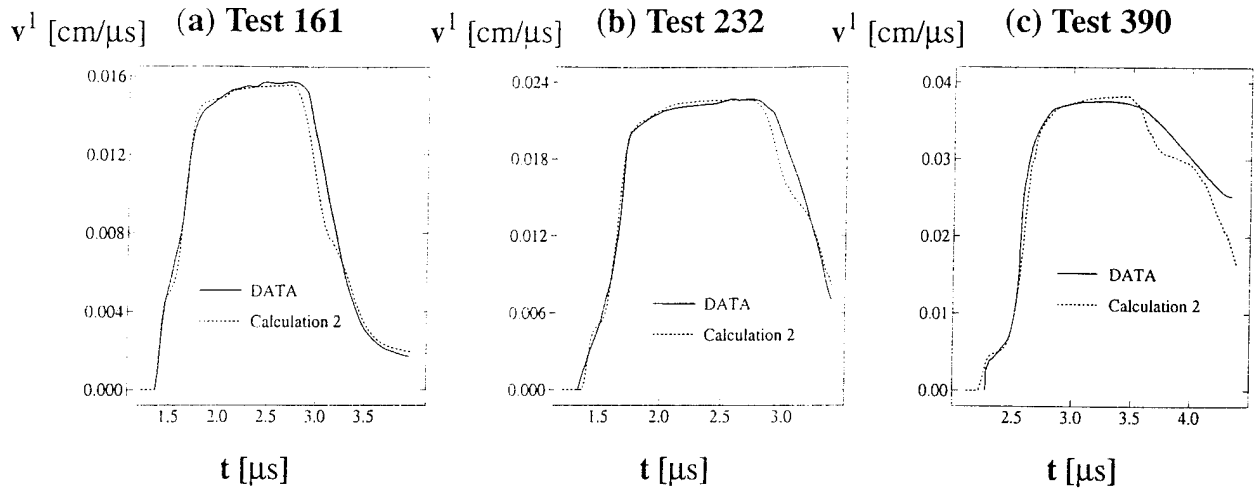
FIGURE 1.5. Comparison of the experimental data and our calculations with the new material model with the new material parameter $C_2 = 0.035$ Mb ms. The plots display the velocity of the right-hand free surface *vs.* time in tests 161, 232, and 390.

the simulations to reproduce the experiments were the same for the two formulations. For our improved model, one of the indirectly inferred material constants required a value different from that used previously. Agreement between simulation and experiment was satisfied, both before and after improvement of the physics model. See Figure 1.5 for the agreement between simulation and experiment, for the corrected theory and the corrected material parameter.

In order to compute plate impact problems in an Eulerian formulation, material boundaries not aligned with mesh boundaries were encountered. To handle this difficulty, a simple form of front tracking was introduced [Wang et al., 1993b]. In order to extend tracking to other waves of interest in plastic deformation problems. a model of shear bands, with jump relations across the shear band is required. We have begun a modeling program to study shear bands. Shear bands arise as an instability in laminar shear deformation. As one portion of the shear layer suffers more plastic deformation, it becomes hotter, hence softer. Thus further shear intensifies in this region, and an instability breaking the laminar behavior is started. Shear bands in metals are very thin (≈ 1 micron), and hence impossible to resolve as part of a macroscopic deformation simulation. They must be modeled. Our model, as presently completed [Glimm et al., 1993b], concerns a fully formed shear band in its inner region. in which heat conduction is in approximate balance with heat formation. A simplified model equation for the evolution of the shear band is

$$\theta_t = k\theta_{yy} = \sigma\dot{\gamma}_\mathrm{p}$$

where θ is temperature, k is thermal conductivity, σ is the dominant component of the shear stress, $\dot{\gamma}$ is the shear strain rate, and the subscript p denotes the plastic component. The key aspect of this equation is the nonlinear source term describing the plastic flow rule, *i.e.*, the heat generated by plastic work. Our expression

$$\dot{\gamma}_\mathrm{p} = \frac{1}{b}\mathrm{sgn}(\sigma)|\sigma|^{1/m}g(\theta)^{-1/m}$$

for this term contains some modeling assumptions. See [Clifton et al., 1984, Wright and Batra, 1985, Wright and Walter, 1987, Walter, 1992] for related studies.

1.4.4. *Object Oriented Numerical Methods.* The increasing power and size of the front tracking code has led to a corresponding increase in the time and effort needed to train new personnel in the use and development of the code. Joint research efforts with the Los Alamos National

Laboratory and the Army Research Laboratory also require the addition of new capabilities in the code such as molecular mixing, elasto-plasticity, and radiation hydrodynamics. These and other upgrades require an improved implementation of the front tracking code using modern object oriented programming techniques. This work has led to improved modularity in the code structure that allows new applications to be inserted more easily. Recent work includes the installation of elasto-plasticity models and multiple fluid mixing capabilities in the front tracking code.

2. PROFESSIONAL ACTIVITIES

2.1. James Glimm.

2.1.1. *Editorial boards.*

- SIAM Review 1989-1997
- Acta Mathematicae Applicandae
- Progress in Mathematical Physics
- Applied Mathematics Letters
- Proceedings American Mathematics Society
- Zeitschrift fur Angewandte Mathematik und Physik
- Journal of Nonlinear Analysis
- Computational Geosciences
- Electronic Research Announcements of the American Mathematical Society
- What's Happening in the Mathematical Sciences
- Scientific Advisor: Los Alamos National Laboratory Preprint Bulletin Board, Computational Methods/Data Analysis/Wavelets/Lattice Gases
- Series Editor: Mathematical Methods in the Life Sciences, World Scientific Publishers, Inc.

2.1.2. *Committee Memberships (Selected).*

- Board on Mathematical Sciences, National Research Council (1988-1994)
- Science Policy Committee, SIAM (1985-1996); Chairman 1988-92
- Program Director, SIAM Activity Group on Geosciences
- Board of Trustees, MSRI (Berkeley) (1989-1994)
- Advisory Board, AHPCRC (Minnesota) (1991-)
- Public Information Resource Committee, Joint Policy Board on Mathematics (1987-)

2.1.3. *Contacts with Industry.* Professor Glimm has initiated and maintained numerous active contacts with industry. The include a Resin Transfer Model project with Northrup-Grumman, reservoir modeling with the Chevron Corporation, semiconductor manufacture with the DawnTech Corporation, and parallel computing projects with the Intel Corporation. Industrial and dual use technologies research began with a survey of potential uses of mathematical modeling in advanced manufacturing and management practices. One application was the problem of geometric pattern recognition for the study of binding sites for the design of pharmaceuticals. Here the large combinatorial complexity of the pattern matching optimization function is the main difficulty. A rapid algorithm was developed for the solution of this problem. The method was compared to X-ray crystallography to determine the degree to which hydrogen bonds alone provide binding specificity for binding of protein on DNA.

2.1.4. *Contact with Army Laboratory Personnel.* Contacts with Drs. Tim Wright and John Walters at the ARL have led to the establishment of the front tracking code used by researchers at Stony Brook at the laboratory. Ongoing collaboration in the modeling of elasto-plastic flows and adiabatic shear bands are being conducted.

Gerald E. Cooper chief of the Advanced Research Projects Office U.S. Army Concepts Analysis Agency has initiated contact with Professor Glimm on the modernization and optimization of the CEM theater combat model. Investigations for possible areas of collaboration are ongoing.

2.2. John W. Grove.

2.2.1. *Editorial boards.*

* Computers and Mathematics with Applications

2.2.2. *Conferences Organized.*

1. Fifth International Conference on Hyperbolic Problems, Theory, Numerics, Applications, University at Stony Brook, Stony Brook NY, June 12-17, 1994
2. Conference in Honor of the Sixtieth Birthday of James Glimm, University at Stony Brook, Stony Brook NY, April 20-22, 1995
3. Fifth International Workshop on the Physics of Compressible Turbulent Mixing, University at Stony Brook, Stony Brook NY, June 12-17, 1995

2.2.3. *Collaboration with Government Laboratories.*

During the period of this grant Grove made several visits to government laboratories, both to the Los Alamos National Laboratory, and the Army Research laboratory. Grove's work at these sights concerns collaboration with laboratory researchers (R. Benjamin, K. Lackner, R. Menikoff, and D. H. Sharp of LANL, J. Walter and T. Wright of ARL) on numerical methods for modeling complex flows. In particular his work at Los Alamos is primarily based on using front tracking to model complex multi-fluid mixing, and my work at ARL is devoted to the development of front tracking methods for modeling elasto-plasticity. Both collaborations with DOE and ARL personnel have been established on a long term and continuing basis. The details of these research projects are described above.

2.2.4. *Contacts with Industry.*

The INTEL corporation has agreed to donate eight nodes for their Paragon parallel supercomputer for use in front tracking simulations of complex mixing.

2.2.5. *National Service.*

1. Member National Science Foundation Review Panel for Small Business Innovation Research Program, September 26, 27 1994
2. Member National Science Foundation Review Panel Early Career Development Program, February 21-23, 1995

2.2.6. *Educational and Human Resources Development.*

During the academic year of 1994/95 Grove supervised four graduate students, B. Boston, M. J. Graham, A. Pass, and S. Tael, two of whom are women. B. Boston will complete his Ph.D. at the end of June 1995, while A. Pass, and S. Tael expect to complete their Ph.D.'s by the end of August 1995. B. Boston has accepted a position as a postdoctoral associate at the University of Stony Brook for the academic year of 1996-97, A. Pass has accepted a position at Equitable Insurance Company as an actuary, S. Tael has applied for a postdoctoral position at the Army Research Laboratory. During the same period Grove co-supervised five postdoctoral students, R. Holmes, X. Lin, K.-M. Shyue, R. Young, and Y. Zeng. R. Holmes, who received his Ph.D. in August 1994 under Grove's supervision, has been awarded an NSF postdoctoral fellowship and will work at New York University during the academic year of 1995-96. K.-M. Shyue received a full time position at the University of Taiwan, and X. Lin, R. Young, and Y. Zeng will continue their postdoctoral positions at Stony Brook for the next academic year.

3. PUBLICATIONS AND TECHNICAL REPORTS

[1] B. Boston, J. W. Grove, L. F. Henderson, R. Holmes, D. H. Sharp, Y. Yang, and Q. Zhang. Shock induced surface instabilities and nonlinear wave interactions. Report No. SUNYSB-AMS-93-20. State Univ. of New York at Stony Brook, 1993. Proceedings of Eleventh Army Conference on Applied Mathematics and Computing.

[2] Y. Deng, J. Glimm, and D. H. Sharp. Mixing and chaotic microstructure. *Los Alamos Science*, 21:124–132, 1993.

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4. Participating Scientific Personnel

4.1. Senior Personnel.
1. James Glimm
2. John W. Grove

4.2. Student Personnel.
1. R. Holmes. Received Ph.D Summer 1994
2. Bin He
3. D. Saltz, Ph.D. expected August 1995
4. S. Tael
5. N. Zsifkov

5. Report of Inventions

No mechanical inventions were created due to work under this grant. Substantial development and improved modeling capabilities have been add to numerical software created under the sponsorship of this grant.

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